7th Int. Symp. "Nanostructures: Physics and Technology"
St Petersburg, Russia, June 14–18, 1999

Symmetry of the GaAs crystal with δ-doping Si layers and its influence on the band structure

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Abstract. The GaAs crystals are shown to lower symmetry from T_d to D_{2d} or C_{2v} when inserting a δ-layer with odd or even number of Si planes respectively. These symmetry changes correspond to uniaxial or plane distortion of the GaAs lattice in the neighbourhood of a δ-layer. The band shifts of GaAs induced by the insertion of δ-layers are estimated.

Introduction

The progress in MBE and MOCVD technologies allowed to fabricate semiconductor heterostructures with a spatial scale comparable with a crystal lattice constant [1]. It has been pointed out [2, 3] that the continuum models (such as envelope-function method, effective-mass method [4] etc.), which proved to be effective for heterostructures with thick layers, failed to describe adequately the physical properties of nanostructures. For heterostructures with thick layers, the validity of continuum models results from translational symmetry in each layer which breaks only at interfaces. As a result, the description of such structures is based on the parameters of constituent bulk crystals.

However, for heterostructures with ultrathin layers (comprising several atomic planes) the translational symmetry along the direction perpendicular to the layers is lost in any individual layer because the thickness of a layer is comparable with the lattice constant. Moreover, interface regions become comparable with a layer thickness. Therefore, to study the properties of such systems we should start with determination of their crystal structure (space group and atomic arrangement within a primitive cell), i.e. to treat them as new crystals with own symmetry.

The performed analysis shows [3] that in superlattices (SL), new periodicity arises along the growth direction accompanied by a change of their point symmetry. In general, the space group and atomic arrangement over the Wyckoff positions in the primitive cell turn out to be functions of the SL growth direction and numbers of monolayers of constituent bulk materials forming the SL. As a result, a symmetry of a SL can be described by one of the 230 (three-dimensional three-periodic) space groups.

In contrast, in δ-doped systems, the periodicity along the direction perpendicular to the layers disappears.

1 Symmetry of the GaAs crystal with Si δ-layers

A GaAs crystal with a Si δ-layer is a 3D system with 2D translational symmetry. The symmetry of such systems is described by one of the 80 diperiodic groups in 3D [5]. The

Table 1. Symmetry of the GaAs crystal with Si δ-layers.

No of Si planes n	Space group G	Point group G_0	Bravais lattice	Atomic arrangement
bulk	T_d^2	T_d	fcc	1a(000)−Ga(T_d); 1c$\left(\frac{1}{4}\frac{1}{4}\frac{1}{4}\right)$-As($T_d$);
1	DG59	D_{2d}	square	1a(000)−$Si_{Ga/As}$(D_{2d}); 2f$\left(\frac{1}{2}\frac{1}{2}z\right)$-Ga/As($C_{2v}$);
	$P\bar{4}m2$			2g$\left(0\frac{1}{2}z\right)$-As/Ga($C_{2v}$)
2	DG23	C_{2v}	primitive	1a(00z)−Si_{Ga}(C_{2v}); 1c$\left(0\frac{1}{2}z\right)$−$Si_{As}$ (C_{2v});
	P2mm		rectangular	1b$\left(0\frac{1}{2}z\right)$-As($C_{2v}$); 1d$\left(\frac{1}{2}\frac{1}{2}z_1\right)$-Ga($C_{2v}$);
				1d$\left(\frac{1}{2}\frac{1}{2}z_2\right)$-Ga($C_{2v}$)
3	DG59	D_{2d}	square	1a(000)-Si_{Ga} (D_{2d}); 2g$\left(0\frac{1}{2}z_1\right)$-$Si_{As}$ (C_{2v});
	$P\bar{4}m2$			2f$\left(\frac{1}{2}\frac{1}{2}z\right)$-Ga($C_{2v}$); 2g$\left(0\frac{1}{2}z_2\right)$-As($C_{2v}$)

typical representatives of the δ-Si:GaAs structure with one and two Si planes constituting a δ-layer are shown in Fig. 1.

We determined that the crystal structure of such a system (space group and arrangement of atoms over the Wyckoff positions) depends on the number n of Si atomic planes in a δ-layer. The results of the analysis are presented in Table 1. The Wyckoff positions and their coordinates follow notations of [5].

Notice, that our analysis is valid for any crystal with a zinc-blende structure including GaN, InN, InAs etc.

From Table 1, one can see that the introduction of one (odd) Si plane reduces the point symmetry of the GaAs bulk crystal from T_d to D_{2d} whereas the introduction of two (even) planes from T_d to C_{2v}. Thus, in the case of odd number of Si planes, the x and y axes are equivalent whereas they become inequivalent for even number of Si planes. For $n = 1$, we have considered two cases: Si substitutes Ga or As (Si_{Ga} or Si_{As}, respectively). In both cases, the symmetry remains the same but Ga and As atoms in adjacent planes interchange their symmetry positions.

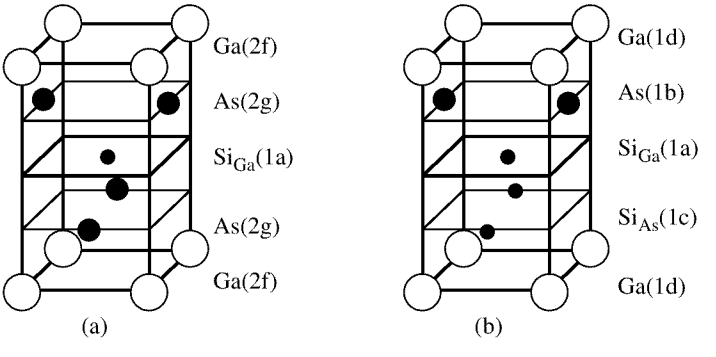

Fig. 1. The crystal structures of the GaAs crystal with one (a) and two (b) Si planes in a δ-layer.

2 Influence of Si δ-layer-induced lattice distortions on band structure

We can see that the introduction of one (odd) Si atomic plane in a bulk GaAs is equivalent (from the point of view of symmetry) to uniaxial deformation of the bulk crystal whereas the introduction of two (even) Si atomic planes corresponds to plane deformation. This modifies the valence (VB) and conduction band (CB) states.

As an example, we estimate the band shifts induced by lattice distortions along the [001] direction due to the insertion of a δ-layer with one Si plane (see Fig. 2). In case of uniaxial deformation, the shifts of conduction band (CB), heavy-hole (HH), light-hole (LH) and spin-orbit split-off (SO) bands measured from the CB bottom and VB top at zero strain (without a δ-layer), ΔE (CB), ΔE (HH) and ΔE (LH,SO), are given by [6]

$$\Delta E(\mathrm{CB}) = \frac{2}{3}E_{\mathrm{H}}, \tag{1a}$$

$$\Delta E(\mathrm{HH}) = -\frac{1}{3}E_{\mathrm{H}} - E_{\mathrm{U}}, \tag{1b}$$

$$\Delta E(\mathrm{LH,SO}) = -\frac{1}{3}E_{\mathrm{H}} - \frac{1}{2}\left[(\Delta - E_{\mathrm{U}}) \mp (9E_{\mathrm{U}}^2 + 2E_{\mathrm{U}}\Delta + \Delta^2)^{1/2}\right] \tag{1c}$$

where $E_{\mathrm{H}} = 2\mathrm{a}[(\mathrm{C}_{11} - \mathrm{C}_{12})/\mathrm{C}_{11}]\epsilon_{\mathrm{Ga/As}}$, $E_{\mathrm{U}} = -\mathrm{b}[(\mathrm{C}_{11} + 2\mathrm{C}_{12})/\mathrm{C}_{11}]\epsilon_{\mathrm{Ga/As}}$; $\epsilon_{\mathrm{Ga/As}}$ is the strain induced by a Si plane substituting Ga or As planes, C_{11} and C_{12} are elastic constants, a and b are hydrostatic and shear deformation potentials, respectively, Δ is spin-orbit split-off energy.

We estimate the strain $\epsilon_{\mathrm{Ga/As}}$ in the neighbourhood of a δ-layer as a relative difference of corresponding covalent tetrahedral radii:

$$\epsilon_{\mathrm{Ga/As}} = (r_{\mathrm{Si}} - r_{\mathrm{Ga/As}})/2r_{\mathrm{Si}}. \tag{2}$$

For GaAs, taking the values of covalent tetrahedral radii ($r_{\mathrm{Si}} = 1.17$ Å, $\mathrm{r_{Ga}} = 1.26$ Å and $r_{\mathrm{As}} = 1.17$ Å) from [7], the values of elastic constants ($\mathrm{C}_{11} = 1.188 \times 10^{12}$ dyn/cm^2, $\mathrm{C}_{12} = 0.538 \times 10^{12}$ dyn/cm^2) and deformation potentials (a = −8.9 eV, b = −1.73 eV) as well as spin-orbit split-off energy ($\Delta = 0.34$ eV) from [6], we obtain the values for band

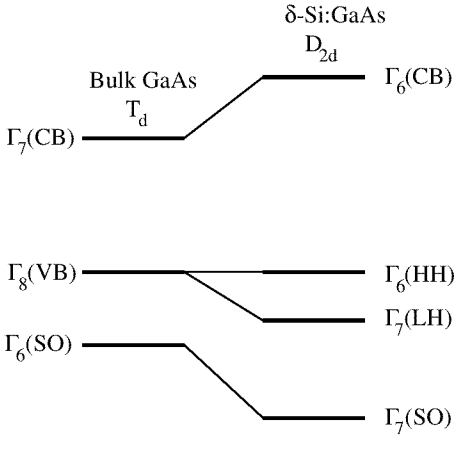

Fig. 2. GaAs band state modification induced by insertion of one Si plane (band shifts correspond to Table 2).

Table 2. CB and VB shifts (in eV) in GaAs regions in the neighbourhood of a δ-layer.

	Si at Ga position	Si at As position
$\epsilon_{Ga/As}$	–0.038	0.0043
E_H	0.374	0.0416
E_U	–0.127	–0.0141
ΔE(CB)	0.249	0.028
ΔE(HH)	0.002	0.002
ΔE(LH)	–0.150	–0.028
ΔE(SO)	–0.571	–0.354

shifts in GaAs regions in the neighbourhood of a δ-layer given in Table 2. Note that the case of even numbers of Si planes is more sophisticated: the plane deformation arises that induces anisotropy in the xy plane.

From the above results, we see that in the case of Si substituting Ga the band gap strongly increases whereas for Si at As sites the band shifts are much smaller. This leads to changes of band populations, mobility and other kinetic coefficients in the neighbourhood of a δ-layer [8]. The lattice distortion extends over tens of lattice constants. Thus, these effects are to be taken into account when analyzing the properties of nanostructures.

Acknoledgements

The authors acknowledge the Russian Ministry of Education Grant 97-5-5.3-19. One of us (PT) wishes to thank the French Embassy in Moscow for the support.

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